

chain nodes :

7 8 9 17 18 19 20 21

ring nodes :

1 2 3 4 5 6 10 11 12 13 14 15

chain bonds :

2-17 5-7 7-8 7-9 9-11 17-18 17-20 18-19 20-21

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15

exact/norm bonds :

1-2 1-6 2-3 2-17 3-4 4-5 5-6 5-7 7-8 7-9 9-11 10-11 10-15
11-12 12-13 13-14 14-15 18-19 20-21

exact bonds :

17-18 17-20

isolated ring systems :

containing 1 : 10 :

G1:O,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 17:CLASS 18:CLASS
19:Atom 20:CLASS 21:Atom

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

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*
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*
*****
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<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>
Uploading structure

L1 STRUCTURE UPLOADED

=> s l1
SAMPLE SEARCH INITIATED 11:19:04 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 135 TO ITERATE

100.0% PROCESSED 135 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
PROJECTED ITERATIONS: 2003 TO 3397
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 11:20:21 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2484 TO ITERATE

100.0% PROCESSED 2484 ITERATIONS 31 ANSWERS
SEARCH TIME: 00.00.01

L3 31 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
 ENTRY SESSION
FULL ESTIMATED COST 166.92 167.13

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FILE COVERS 1907 - 2 Oct 2005 VOL 143 ISS 15
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=> s l3

L4 1 L3

=> d l4 bib abs hitstr

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2005 ACS on STN

Full Text

AN 2004:453187 CAPLUS

DN 141:7141

TI A preparation of piperazine derivatives, useful as 17 β -hydroxysteroid dehydrogenase type 3 inhibitors

IN Paruch, Kamil; Guzi, Timothy J.

PA Schering Corporation, USA

SO PCT Int. Appl., 49 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004046111	A1	20040603	WO 2003-US36203	20031114
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LU, LV, MA, MD, MG, MK, MN, MX, MZ, NI, NO, NZ, PG, PH, PL, PT, RO, RU, SC, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UZ, VC, VN, YU, ZA, ZM				
	RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2506290	AA	20040603	CA 2003-2506290	20031114
	US 2004127503	A1	20040701	US 2003-713828	20031114
	EP 1562901	A1	20050817	EP 2003-783382	20031114
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PRAI	US 2002-427263P	P	20021118		
	WO 2003-US36203	W	20031114		
OS	MARPAT 141:7141				
GI					

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to a prepn. of piperazine derivs. of formula I [wherein: X is CH or N; Z is O or NH, N-alkyl, or N-aryl, etc.; R1 and R2 are independently selected from (un)substituted (hetero)aryl, (hetero)arylalkyl; R3 is H, OH, alkoxy, aryloxy, etc.; R4 is H, (cyclo)alkyl, (hetero)aryl, etc.; R5 is C(O)R6 or SO2R6; R6 is alkyl,

(hetero)aryl, (hetero)arylalkyl, (un)substituted amine], useful as inhibitors of type 3 17 β -hydroxysteroid dehydrogenase. The invention compds. are claimed to be useful for the treatment, prevention, inhibition, or amelioration of diseases such as prostate cancer, acne, and androgenic alopecia, etc. The invention compds. exhibited a range of 17 β -hydroxysteroid dehydrogenase type 3 binding activity from about 0.005 nM to 10 nM. For instance, piperazine deriv. II was prepd. via amination of phenyl(trifluoromethylphenyl)methanol by (S)-2-tert-butylpiperazine (example 7) and subsequent reaction of the obtained piperazine deriv. III and piperidine deriv. IV (example 15).

IT 696644-18-5P 696644-21-0P 696644-24-3P

696644-28-7P 696644-32-3P 696644-36-7P

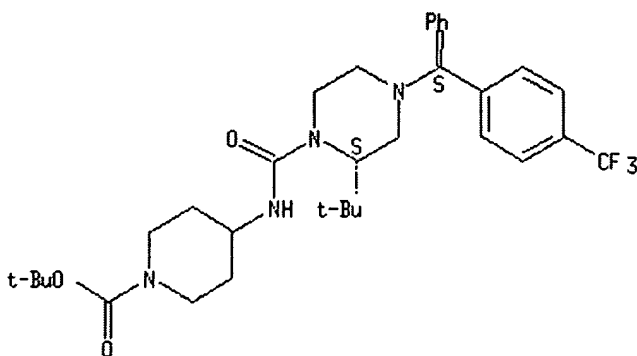
RL: PAC (Pharmacological activity); PUR (Purification or recovery); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 17 β -hydroxysteroid dehydrogenase type 3 inhibitors for the treatment of androgen-dependent diseases)

RN 696644-18-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[(S)-phenyl[4-(trifluoromethyl)phenyl]methyl]-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

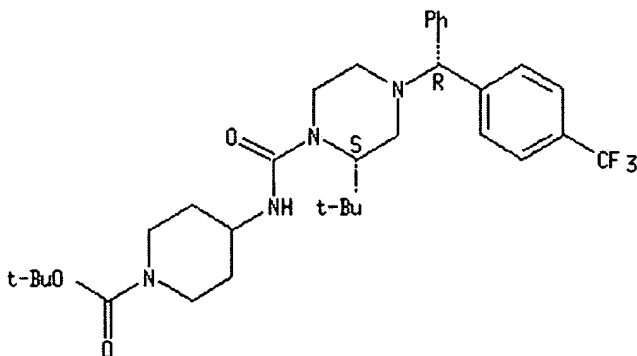
Absolute stereochemistry.



RN 696644-21-0 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[(R)-phenyl[4-(trifluoromethyl)phenyl]methyl]-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

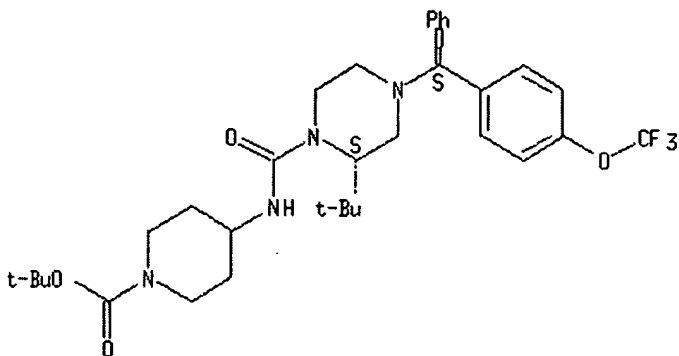


RN 696644-24-3 CAPLUS

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CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[(S)-phenyl[4-(trifluoromethoxy)phenyl]methyl]-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

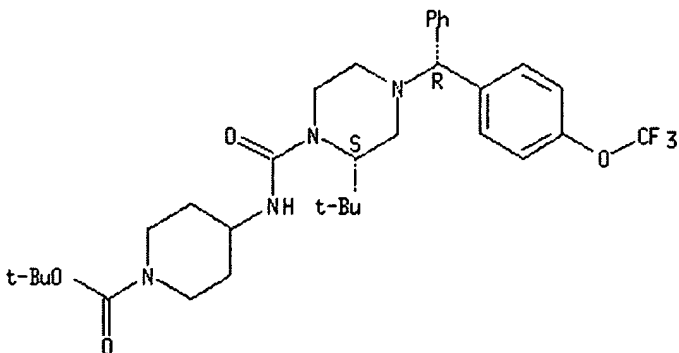
Absolute stereochemistry.



RN 696644-28-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[(R)-phenyl[4-(trifluoromethoxy)phenyl]methyl]-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

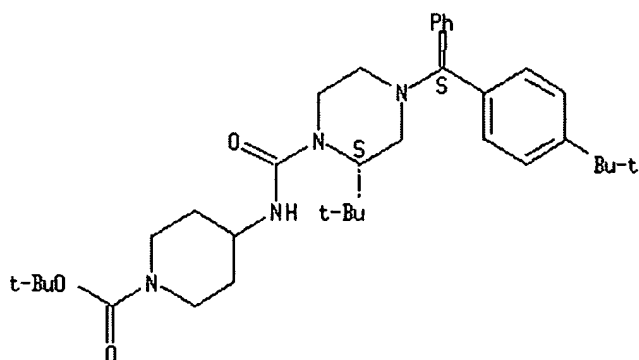
Absolute stereochemistry.



RN 696644-32-3 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[(S)-[4-(1,1-dimethylethyl)phenyl]phenylmethyl]-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

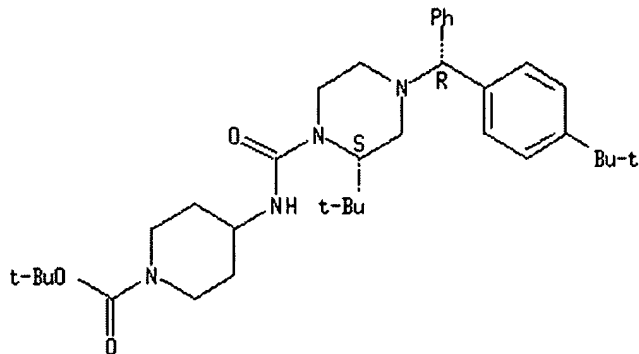
Absolute stereochemistry.



RN 696644-36-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[(R)-[4-(1,1-dimethylethyl)phenyl]phenylmethyl]-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 696643-77-3P 696643-81-9P 696643-85-3P
 696643-88-6P 696643-92-2P 696643-96-6P
 696644-00-5P 696644-12-9P 696644-15-2P
 696644-40-3P 696644-45-8P 696644-50-5P
 696644-54-9P 696644-58-3P 696644-60-7P
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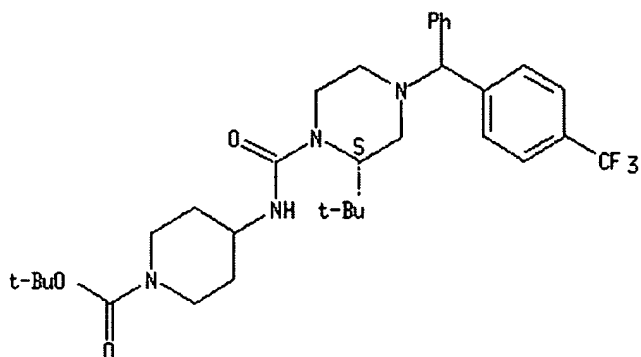
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 17 β -hydroxysteroid dehydrogenase type 3 inhibitors for the treatment of androgen-dependent diseases)

RN 696643-77-3 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[phenyl[4-(trifluoromethyl)phenyl]methyl]-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

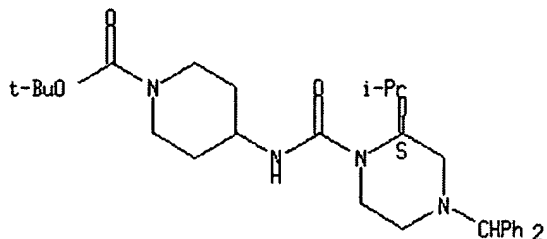
Absolute stereochemistry.



RN 696643-81-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-4-(diphenylmethyl)-2-(1-methylethyl)-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI)
(CA INDEX NAME)

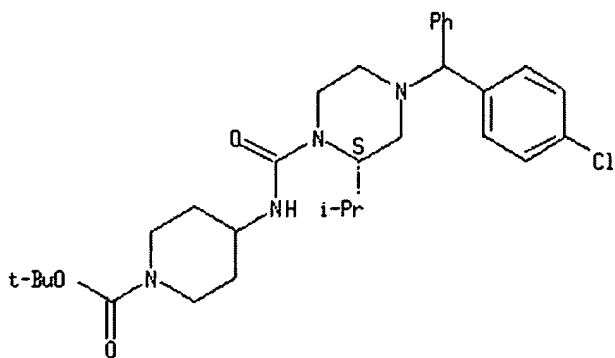
Absolute stereochemistry.



RN 696643-85-3 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-4-[(4-chlorophenyl)phenylmethyl]-2-(1-methylethyl)-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

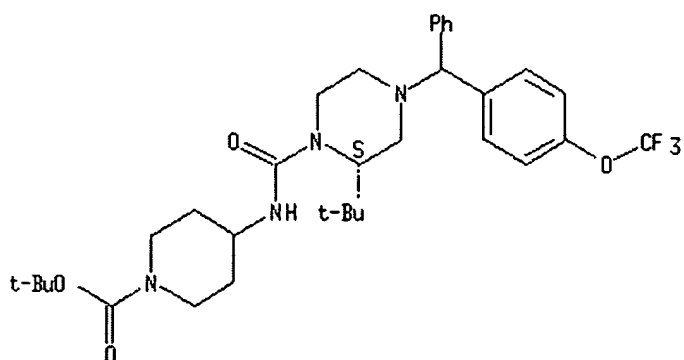
Absolute stereochemistry.



RN 696643-88-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[phenyl[4-(trifluoromethoxy)phenyl]methyl]-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

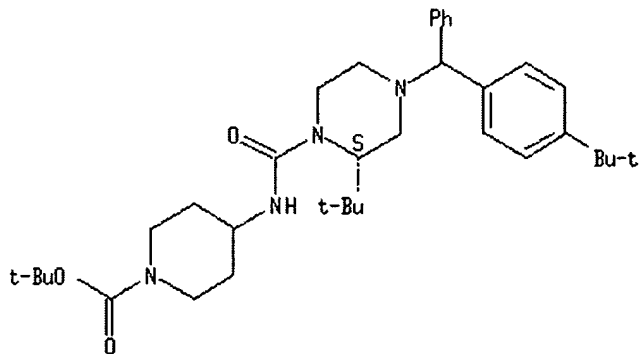
Absolute stereochemistry.



RN 696643-92-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-2-(1,1-dimethylethyl)-4-[[4-(1,1-dimethylethyl)phenyl]phenylmethyl]-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

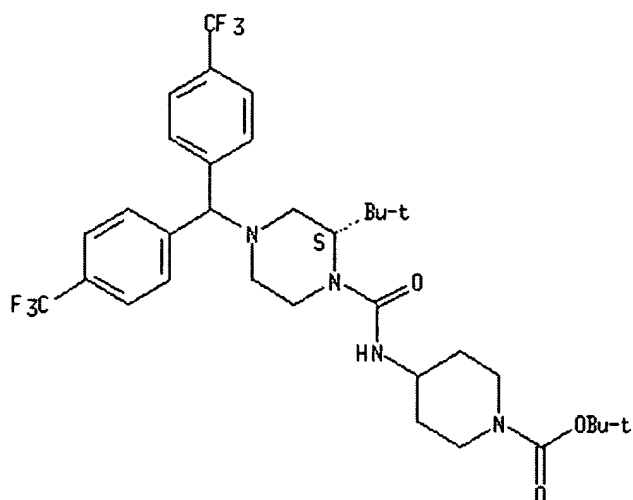
Absolute stereochemistry.



RN 696643-96-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-4-[bis[4-(trifluoromethyl)phenyl]methyl]-2-(1,1-dimethylethyl)-1-piperazinyl]carbonyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

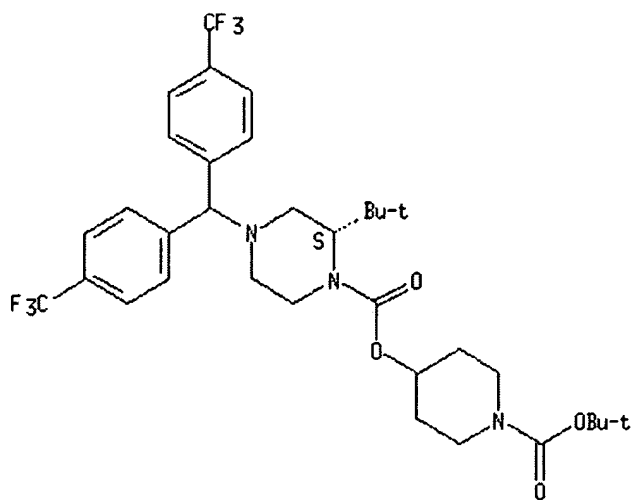
Absolute stereochemistry.



RN 696644-00-5 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[bis[4-(trifluoromethyl)phenyl]methyl]-2-(1,1-dimethylethyl)-, 1-[(1,1-dimethylethoxy)carbonyl]-4-piperidinyl ester, (2S)-(9CI) (CA INDEX NAME)

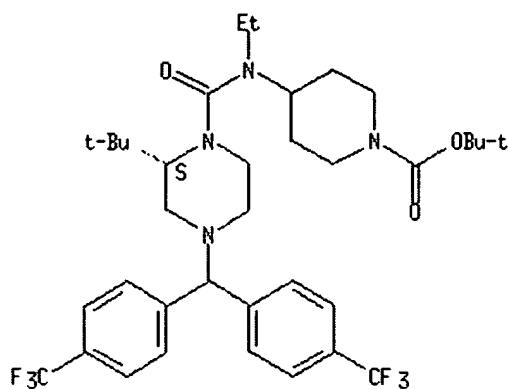
Absolute stereochemistry.



RN 696644-12-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-4-[bis[4-(trifluoromethyl)phenyl]methyl]-2-(1,1-dimethylethyl)-1-piperazinyl]carbonyl]ethylamino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

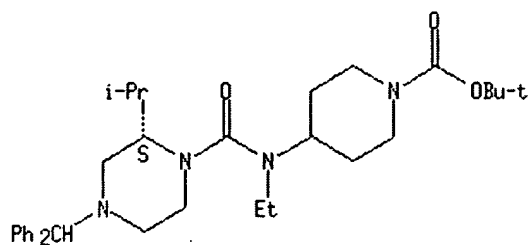
Absolute stereochemistry.



RN 696644-15-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[(2S)-4-(diphenylmethyl)-2-(1-methylethyl)-1-piperazinyl]carbonyl]ethylamino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

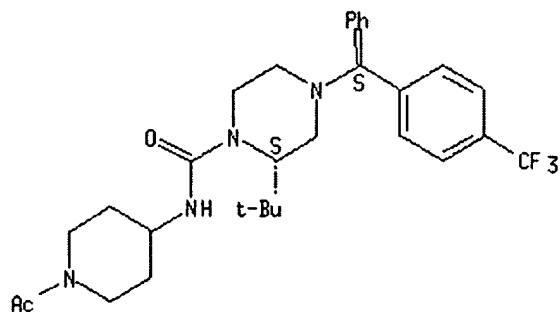
Absolute stereochemistry.



RN 696644-40-3 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidiny)-2-(1,1-dimethylethyl)-4-[(S)-phenyl[4-(trifluoromethyl)phenyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

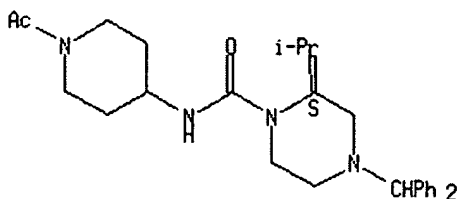
Absolute stereochemistry.



RN 696644-45-8 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidiny)-4-(diphenylmethyl)-2-(1-methylethyl)-, (2S)- (9CI) (CA INDEX NAME)

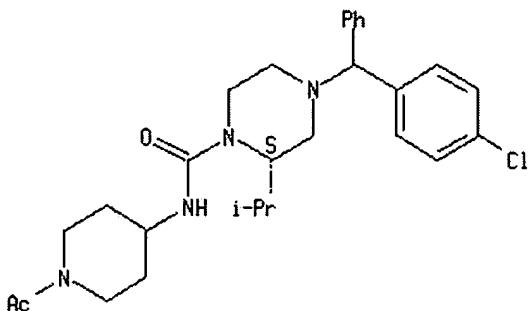
Absolute stereochemistry.



RN 696644-50-5 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidiny)-4-[(4-chlorophenyl)phenylmethyl]-2-(1-methylethyl)-, (2S)- (9CI) (CA INDEX NAME)

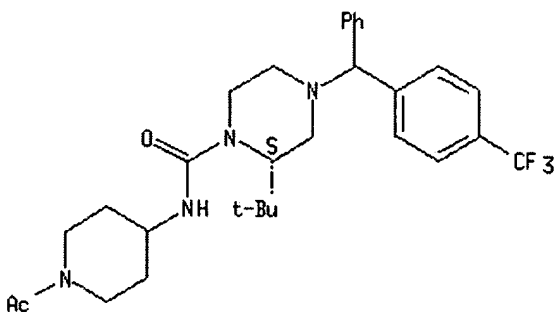
Absolute stereochemistry.



RN 696644-54-9 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidiny)-2-(1,1-dimethylethyl)-4-[phenyl[4-(trifluoromethyl)phenyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

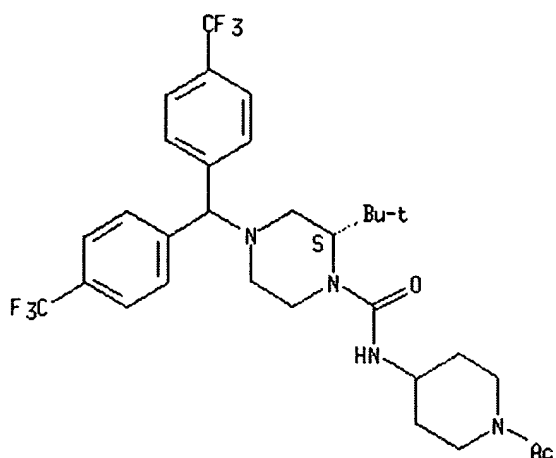
Absolute stereochemistry.



RN 696644-58-3 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidiny)-4-[bis[4-(trifluoromethyl)phenyl]methyl]-2-(1,1-dimethylethyl)-, (2S)- (9CI) (CA INDEX NAME)

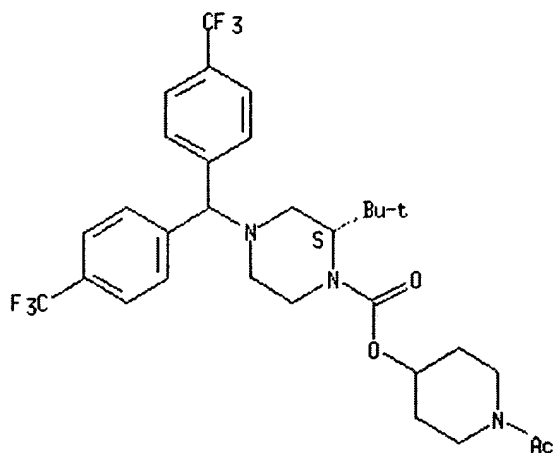
Absolute stereochemistry.



RN 696644-60-7 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[bis[4-(trifluoromethyl)phenyl]methyl]-2-(1,1-dimethylethyl)-, 1-acetyl-4-piperidinyl ester, (2S)- (9CI) (CA INDEX NAME)

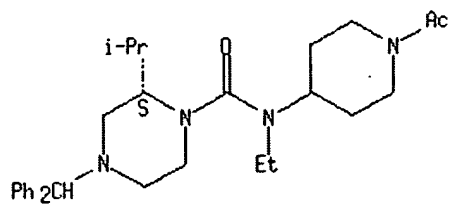
Absolute stereochemistry.



RN 696644-64-1 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-4-(diphenylmethyl)-N-ethyl-2-(1-methylethyl)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

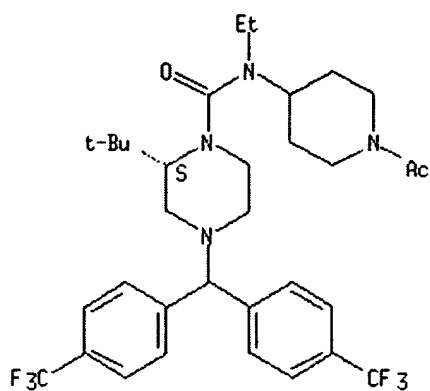


RN 696644-66-3 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-4-[bis[4-(trifluoromethyl)phenyl]methyl]-2-(1,1-dimethylethyl)-N-ethyl-, (2S)- (9CI) (CA INDEX NAME)

(9CI) (CA INDEX NAME)

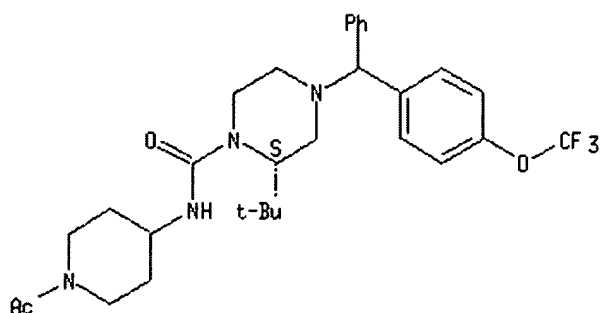
Absolute stereochemistry.



RN 696644-68-5 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidiny)-2-(1,1-dimethylethyl)-4-[phenyl[4-(trifluoromethoxy)phenyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

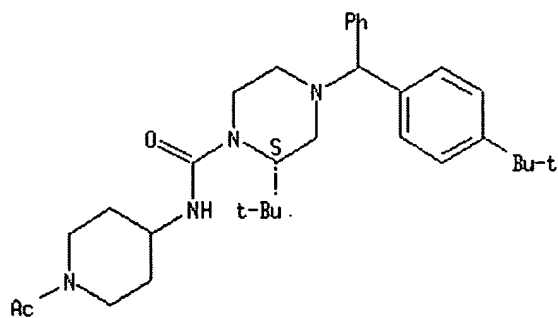
Absolute stereochemistry.



RN 696644-70-9 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidiny)-2-(1,1-dimethylethyl)-4-[4-(1,1-dimethylethyl)phenyl]phenylmethyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

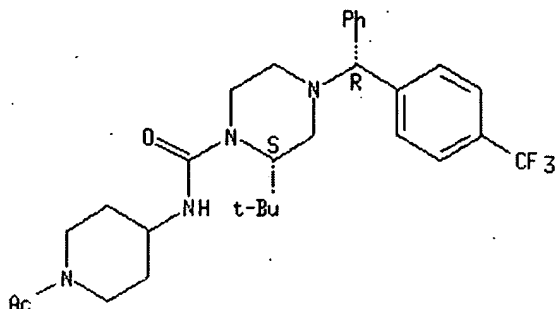


RN 696644-72-1 CAPLUS

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CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-2-(1,1-dimethylethyl)-4-[(R)-phenyl[4-(trifluoromethyl)phenyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

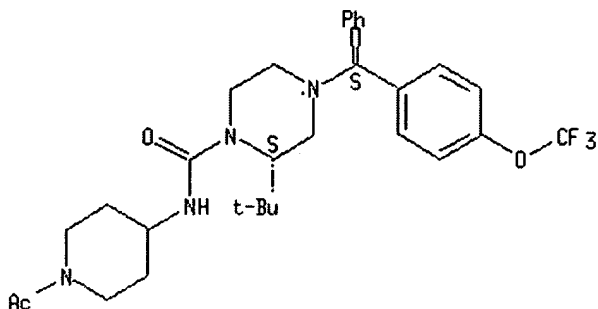
Absolute stereochemistry.



RN 696644-78-7 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-2-(1,1-dimethylethyl)-4-[(S)-phenyl[4-(trifluoromethoxy)phenyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

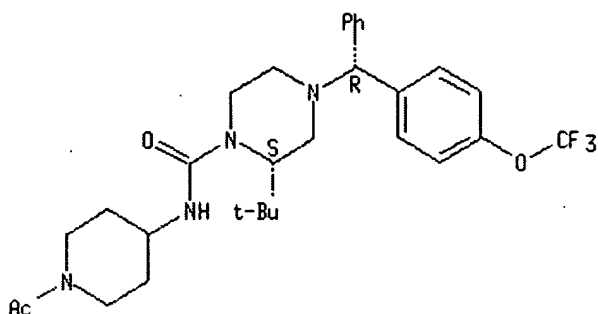
Absolute stereochemistry.



RN 696644-82-3 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-2-(1,1-dimethylethyl)-4-[(R)-phenyl[4-(trifluoromethoxy)phenyl]methyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

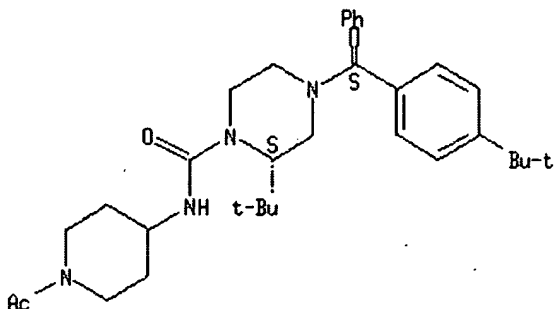


RN 696644-87-8 CAPLUS

STN Columbus

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-2-(1,1-dimethylethyl)-4-[(S)-[4-(1,1-dimethylethyl)phenyl]phenylmethyl]-, (2S)- (9CI) (CA INDEX NAME)

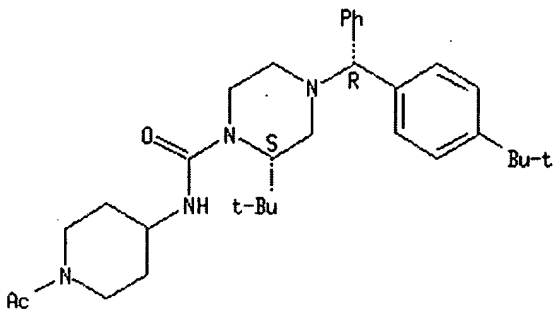
Absolute stereochemistry.



RN 696644-92-5 CAPLUS

CN 1-Piperazinecarboxamide, N-(1-acetyl-4-piperidinyl)-2-(1,1-dimethylethyl)-4-[(R)-[4-(1,1-dimethylethyl)phenyl]phenylmethyl]-, (2S)- (9CI) (CA INDEX NAME)

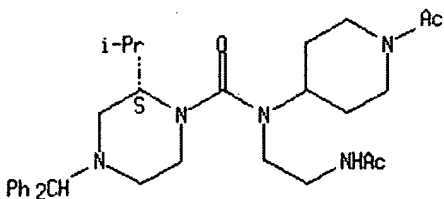
Absolute stereochemistry.



RN 696644-99-2 CAPLUS

CN 1-Piperazinecarboxamide, N-[2-(acetylamino)ethyl]-N-(1-acetyl-4-piperidinyl)-4-(diphenylmethyl)-2-(1-methylethyl)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> file caold
COST IN U.S. DOLLARS

SINCE FILE ENTRY	TOTAL SESSION
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STN Columbus

FULL ESTIMATED COST	5.39	172.52
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-0.73	-0.73

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 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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